

2,3,4-Trimethylpentane
565-75-3 | DTXSID6060343

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.15e-05 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.62e-01

Confidence level: 6.56e-01

Nearest Neighbors from the Training Set

Image not found

2,3,4-Trimethylpentane

Measured: 2.01e-05

Predicted: 1.15e-05

Image not found

Hexane, 2,2-dimethyl-

Measured: 1.75e-06

Predicted: 8.30e-06

Image not found

2,2,4-Trimethylpentane

Measured: 1.96e-05

Predicted: 1.08e-05

Image not found

(3S)-2,2,3-Trimethylpentane

Measured: 2.10e-05

Predicted: 1.09e-05